

Klein paradox for arbitrary spatio-temporal scalar potential and Josephson-like current in graphene

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We derive the exact time evolution according to the Dirac-Weyl equation, describing a monolayer of graphene, in the presence of a scalar potential $U(x, t)$ of arbitrary spatial and temporal dependence at normal incidence, $p_y = 0$. This solution shows that the Klein paradox (the absence of backscattering) persists even for arbitrary temporal modulations of the barrier. Moreover, we identify an unusual oscillating current j_y running along the barrier, despite of the vanishing momentum in y -direction. This current exhibits resemblance to the Josephson current in superconductors, including the occurrence of Shapiro steps and its sine-like dependence on the phase difference of wave functions.

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The growing interest to graphene, see e.g. Ref. 1, 2, is stimulated by many unusual and sometimes counterintuitive properties of this two dimensional material. Indeed, graphene supplies charge carriers exhibiting the pseudo-relativistic dynamics of massless Dirac fermions. One example of the unusual dynamics of electrons and holes in graphene is the Klein tunneling phenomenon [3] which occurs with unit probability through arbitrarily high and thick barriers at perpendicular incidence, irrespective of the particle energy, in accordance with experiment [4]. In consequence, the question arose of how to control the electron motion in graphene and hence boosted detailed studies of Dirac fermions under the influence of various forms of scalar [5–12] or vector [13] potentials.

So far, lots of works were devoted to studies of graphene subject to static periodic electric fields, since these structures known as graphene superlattices [5, 6] allow controlling both spectrum and transport properties of electrons in graphene. For instance, it was shown [6] that 1D graphene superlattices have a deep analogy with photonic crystals formed by alternating right-handed and left-handed transparent media, similar as the earlier stated analogy [7] of a p-n junction in graphene to a Veselago lens. Superlattices of electrostatic periodic potentials can be used to collimate the directional spread of electron beams in graphene [8] so that waves of zero transverse momentum will dominate transport properties.

Applying a time-dependent laser field to a pristine graphene sample opens an alternative and efficient way [9–11] to control spectrum and transport properties of graphene samples. It has been shown that changing the time dependence of laser fields can mimic [10] the influence of any electrostatic graphene superlattices on the electron spectrum in graphene. Studies of how electron transport in graphene is affected by *time-and-space dependent potentials* are yet limited.

For example, it was shown [10] that Dirac fermions in graphene superlattices can acquire an effective mass pro-

portional to the frequency of an applied laser field, accompanied with an exponential suppression of chiral tunneling even for perpendicular incidence upon the barrier, similar as an *ac*-electric field directed parallel to the barrier [11], in stark contrast to Klein tunneling occurring in the absence of the laser field. The question arises whether time-dependent modulations of a electrostatic barrier itself would generate backscattering or not. In this Letter we shall answer this question and further demonstrate novel transport phenomena occurring for general space-time dependent potentials. We focus on a geometry exhibiting the most pronounced Klein paradox, at vanishing transverse momentum ($p_y = 0$) parallel to a barrier, taking the barrier as homogeneous along the y -direction. We present the general solution of the Dirac equation for a scalar potential $U(x, t)$ of *any* spatial and temporal dependencies. For this case we demonstrate unit transmission probability, thus, generalizing the Klein paradox for arbitrary time dependence in $U(x, t)$. Secondly, we discover an oscillating current j_y *along* the barrier, which in view of $p_y = 0$ seems counter intuitive. This current bears resemblance to the Josephson current in superconductors and we demonstrate even similar properties, such as Shapiro steps for properly chosen frequencies. Experimental test of our predictions should be within reach of present day nanostructure design on graphene [12].

Model.— The honeycomb lattice of graphene engenders two copies, $\tau_z = \pm 1$, of Dirac-Weyl Hamiltonians [14]

$$H_0 = v_F [\tau_z \sigma_x \hat{p}_x + \sigma_y \hat{p}_y], \quad (1)$$

centered about two inequivalent Dirac points (“valleys”) K and K' at corners of the hexagonal first Brillouin zone where electron-hole symmetric bands touch; the Pauli matrices $\sigma_{x,y,z}$ act on two-component spinors representing sublattice amplitudes, exhibiting opposite Fermion helicities, $\cdot p/p = \pm 1$. $SU(2)$ rotations with respect to the vector τ of three Pauli matrices allow to continuously transform both copies into one another [15] which

motivated the terminus “valleytronics” for isospin manipulations based on eigenstates to τ_z , Ref. 16, in analogy to the well-known research area of spintronics [17]. Proposals exist to valley polarize carriers, by means of nanoribbons terminated by zig-zag edges [16, 18, 19], by exploiting trigonal warping at elevated energies [20], or by absorbing magnetic textures [21].

Below, we focus on valley polarized situations. Indeed, smooth electromagnetic or disorder potentials do not couple the two valleys [22] so that calculations can be done independently, for either $\tau_z = +1$ or $\tau_z = -1$. Including now the barrier potential $U(x, t) = \hbar W(x, t)$ the Dirac equation becomes

$$\begin{aligned} v_F(\tau_z \hat{p}_x - i\hat{p}_y)\Psi_B + \hbar W(x, t)\Psi_A &= i\hbar \frac{\partial \Psi_A}{\partial t} \\ v_F(\tau_z \hat{p}_x + i\hat{p}_y)\Psi_A + \hbar W(x, t)\Psi_B &= i\hbar \frac{\partial \Psi_B}{\partial t}, \end{aligned} \quad (2)$$

where wave functions Ψ_A, Ψ_B describe electrons on either of the triangular graphene sublattices, v_F is the Fermi velocity, and the momentum operator is defined as $(\hat{p}_x, \hat{p}_y) = (-i\hbar\partial/\partial x, -i\hbar\partial/\partial y)$. This equation has been solved analytically for time-independent potentials either by matching [3] of wave functions for rectangular barriers, or by the WKB method [23–25] for smooth barriers. Additional time dependent harmonic oscillations have been considered of gate voltages on either side of the rectangular barrier [26], or of an electric field parallel to the barrier [11] or in resonance approximation [10]. In the two latter cases a dynamical gap opens which can suppress even perpendicular ($p_y = 0$) tunneling.

Our goal here is to obtain the exact solution of eq. (2) for $p_y = 0$ and arbitrary potential $W(x, t)$ acting at positive times, i.e. $W(x, t < 0) = 0$. In this case, the wave functions Ψ_A and Ψ_B depend on time t and the coordinate x across the barrier, but not on the y -coordinate. This simplifies (2) to read

$$\begin{aligned} -iv_F\tau_z \frac{\partial \Psi_B}{\partial x} + W(x, t)\Psi_A &= i\hbar \frac{\partial \Psi_A}{\partial t} \\ -iv_F\tau_z \frac{\partial \Psi_A}{\partial x} + W(x, t)\Psi_B &= i\hbar \frac{\partial \Psi_B}{\partial t}. \end{aligned} \quad (3)$$

Exact solution.— To solve (3) we use the Ansatz

$$\psi_{\pm}(x, t) = \frac{1}{2} \begin{pmatrix} e^{iS_{\pm}(x, t)} \\ \pm \tau_z e^{iS_{\pm}(x, t)} \end{pmatrix} \quad (4)$$

where the sign \pm distinguishes left and right propagating solutions. Inserting (4) into (3) results in

$$\partial_t S_{\pm}(x, t) \pm v_F \partial_x S_{\pm}(x, t) + W(x, t) = 0. \quad (5)$$

This first order partial differential equation can be solved by the method of characteristics [27], according to which the vector $(1, \pm v_F, -W)$ is tangent to the solution S_{\pm} ,

yielding

$$S_{\pm}(x, t) = S_{\pm}^{(0)}(x \mp v_F t, 0) - \int_0^t dt' W(x \mp v_F(t-t'), t') \quad (6)$$

explicitly in terms of $W(x, t)$. In view of (4) the term $S_{\pm}^{(0)}(x, 0)$ describes the initial wave function $\psi_{\pm}(x, 0)$ at time $t = 0$ which, in the absence of the barrier at $t < 0$, can be, e.g., a plane wave of wave number k in the x -direction, $S_{\pm}^{(0)}(x, 0) = \pm kx$, or some wave packets. Then eq. (6), together with (4), describes the full solution for $t > 0$

$$\begin{aligned} \psi(x, t) &= a_+(x - v_F t) \begin{pmatrix} 1 \\ \tau_z \end{pmatrix} e^{-i \int_0^t dt' W(x - v_F(t-t'), t')} \\ &+ a_-(x + v_F t) \begin{pmatrix} 1 \\ -\tau_z \end{pmatrix} e^{-i \int_0^t dt' W(x + v_F(t-t'), t')} \end{aligned} \quad (7)$$

where $a_{\pm}(x) = e^{iS_{\pm}^{(0)}(x)} = [\Psi_A(x, t = 0) \pm \tau_z \Psi_B(x, t = 0)]/2$ encodes the initial condition. In particular, if the wave packet is initially purely right moving, $a_- = 0$, according to (7), it continues propagating to the right at times $t > 0$ with undistorted density distribution $|a_+(x - v_F t)|^2$ without reflection, acquiring at most a phase factor due to the time dependent barrier. However, the situation becomes much more intriguing when we consider a superposition of left and right movers.

Josephson-like current.— Now we evaluate the current density

$$\begin{aligned} j_x(x, t) &= v_F \psi^*(x, t) \tau_z \sigma_x \psi(x, t) \\ j_y(x, t) &= v_F \psi^*(x, t) \sigma_y \psi(x, t) \end{aligned} \quad (8)$$

for $p_y = 0$. A very nontrivial result occurs if we consider a linear superposition

$$\psi(x, t) = \alpha_+ \psi_+(x, t) + \alpha_- \psi_-(x, t) \quad (9)$$

of the right and left moving solutions, ψ_+ and ψ_- , obtained above, eqs. (4) and (6), assuming that $|\alpha_+|^2 + |\alpha_-|^2 = 1/2$. Note, that an initial density peak arising from some voltage pulse will generally contain simultaneously left and right moving amplitudes.

For the x -component of the current density, flowing perpendicular to the barrier, we find

$$j_x(x, t) = \frac{v_F}{2} (|\alpha_+ a_+(x - v_F t)|^2 - |\alpha_- a_-(x + v_F t)|^2), \quad (10)$$

which is completely defined by the initial conditions and is *independent* of $W(x, t)$. An initially purely right moving wave packet, $a_- = 0$ is again seen to generate an undistorted current density peak $j_x = v_F |a_+(x - v_F t)|^2/2$ moving at v_F towards the right. According to (10), right and left movers in the initial wave will just add their contributions to the current density of opposite sign. Once more, this confirms the finding of perfect Klein tunneling

through a barrier $U(x, t)$ of any space and time dependence. Furthermore, the current j_x does not depend on τ_z , giving the same contribution from both valleys K and K' . Regarding the current normal to the barrier we find no unusual effects arising from the superposition of right and left moving amplitudes.

Surprisingly, although we consider electron momenta with $p_y = 0$, we find a nonzero value for j_y parallel to the barrier,

$$j_y(x, t) = \tau_z v_F |\alpha_+(x - v_F t) \alpha_-(x + v_F t)| \times \text{Im}(\alpha_+ \alpha_-^* e^{i(S_+(x, t) - S_-(x, t))}). \quad (11)$$

Here, we define $S_\pm = \text{Re}(\mathcal{S}_\pm)$. This equation can be rewritten as

$$j_y(x, t) = \tau_z v_F |\alpha_+ a_+(x, t)| |\alpha_- a_-(x, t)| \times \sin[S_+(x, t) - S_-(x, t) + \phi] \quad (12)$$

with $\phi = \arg(\alpha_+ \alpha_-^*)$. While eq. (12) vanishes for unidirectional wave packets since then either α_+ or α_- is zero, $j_y \neq 0$ for superpositions of left and right moving fermions. It is this superposition which causes the qualitatively new phenomenon of a current *along* the barrier, exhibiting striking properties. The sine-dependence in (12) is reminiscent of the Josephson effect where it originates from the spatial overlap of superconducting order parameters in the contacts of a Josephson junction. In contrast to its x -component, the y -component of the current manifests a nontrivial space and time dependence. The latter also depends on τ_z . Therefore, the best way to observe j_y is to prepare a valley-polarized system. For non- or partly polarized situations one should add the current contribution from the second valley, yielding a total current $j_y(x, t) = j_y^K(x, t) + j_y^{K'}(x, t)$ where j_y^K and $j_y^{K'}$ refer to states near K and K' points, respectively. Notice, that a contribution from the other Dirac point K' can compensate the current from K so that j_y would allow to measure the degree of valley polarization in a graphene sample. However, even without valley polarization, the current fluctuations in y -direction,

$$\langle j_y^2 \rangle - \langle j_y \rangle^2 = v_F^2 [1 - |\alpha_+|^2 |\alpha_-|^2 \times \sin^2(S_+(x, t) - S_-(x, t) + \phi)] \quad (13)$$

do not depend on τ_z , and therefore *remain nonzero*.

Spatio-temporal dependence of j_y .— To substantiate this effect we now investigate specific examples for potentials $W(x, t)$ and the analogy between the current j_y and a Josephson current for the valley-polarized situation, $\tau_z = 1$. Let us consider the two potentials $W_1(x) = W_0 x/L$ and $W_2(x) = W_0 \cos(x/L)$, both with characteristic length L and amplitude W_0 . We consider periodic modulations in both cases with frequency ω so that $\overline{W_{1,2}} = 0$ vanishes on time average. As initial condition we assume a superposition of right and left propagating plane waves, $S_\pm^{(0)} = \pm kx$.

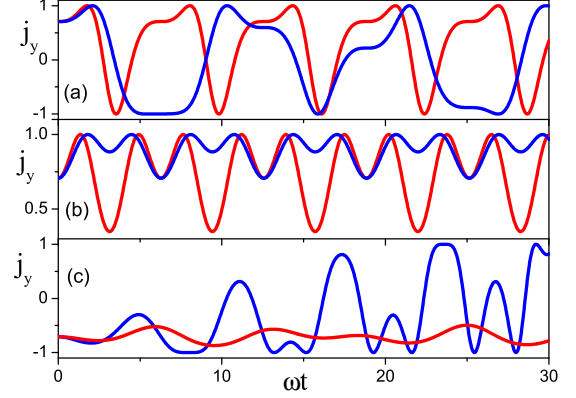


FIG. 1: (Color online) (a) Current j_y (measured in units $j_y^{\max} = v_F |\alpha_+ \alpha_-|$) along the barrier versus time, for the potential $W_1^{(1)}$, see text, $kx + \phi/2 = \pi/8$, and $W_0 v_F / (L \omega^2) = 1/\pi$ (blue line) and $W_0 v_F / (L \omega^2) = 1/2$ (red line), assuming a valley-polarized situation. For “Shapiro-step” conditions periodic oscillations can be seen (red curve), while, away from this condition, aperiodic oscillations occur. (b) The same as (a) but for $W_1^{(2)}$ potentials. This yields periodic solutions with a nonzero *dc*-current for any W_0 ($W_0 v_F / (L \omega^2) = 1/\pi$ (blue) or $W_0 v_F / (L \omega^2) = 1/2$ (red)) and no aperiodic regimes occur. (c) The same as in (a) but for potential $W_2^{(1)}$, $x = \pi L/2$, $k = 0$, $W_0 L / v_F = 0.1$, and frequencies $\omega = (\pi/2)(v_F/L)$ (red curve) and $\omega = v_F/L$ (blue curve). In both cases aperiodic oscillations occur. For the matching condition $\omega = v_F/L$ (blue curve) a considerable enhancement followed by a saturation of the amplitude of the current oscillations occurs, while away of this resonance weak oscillations are not amplified.

Substituting time-dependent potential $W_1^{(1)}(x, t) = W_0(x/L) \sin \omega t$ in eq. (6) and then using eq. (12), we derive

$$j_y(x, t) = v_F |\alpha_+| |\alpha_-| \sin 2 \left[kx + \frac{W_0 v_F}{L} \left(\frac{t}{\omega} - \frac{\sin \omega t}{\omega^2} \right) + \frac{\phi}{2} \right] \quad (14)$$

for this particular potential. This equation can be rewritten as a sum

$$j_y(x, t) = v_F |\alpha_+| |\alpha_-| \sum_{n=0}^{\infty} J_n \left(\frac{2W_0 v_F}{\omega^2 L} \right) \times \sin \left(2kx + \frac{2W_0 v_F t}{\omega L} + n\omega t + \phi \right) \quad (15)$$

using Bessel functions J_n . The last equation indicates that at $\omega = \omega_n$ with

$$\omega_n = \sqrt{2W_0 v_F / (Ln)}, \quad n \in N \quad (16)$$

and integer n , the y -component of the current shows a peculiarity similar to the so-called Shapiro steps [28] of a Josephson junction. As seen in Fig. 1a, the frequencies $\omega = \omega_n$ generate periodic oscillations, which,

again as in the case of Shapiro-steps, exhibit a nonzero dc -component in the current at given x . In view of eqs. (14,15) the overall dc -current vanishes after averaging over x . When modulating the potentials $W_1^{(1)}$ with $\omega \neq \omega_n$ results in aperiodic oscillations and zero dc -component.

The phase shifted modulation $W_1^{(2)}(x, t) = W_0(x/L) \cos \omega t$ yields

$$j_y(x, t) = v_F |\alpha_+| |\alpha_-| \sin 2 \left[kx + \frac{2W_0 v_F}{\omega^2 L} \sin^2 \frac{\omega t}{2} + \frac{\phi}{2} \right] \quad (17)$$

without a term proportional to t in the square bracket argument of the sine-function, cf. eq. (14), and thus without similarity to Shapiro steps in Josephson junctions. The oscillations of j_y generated by $W_1^{(2)}$ are always periodic and with non-zero dc -component as seen in Fig. 1b. The magnitude of this dc -current allows to directly measure the degree of valley polarization as needed for future valleytronics. In the limit $\omega \rightarrow 0$ both versions for W_1 become time-independent.

The second choice, $W_2^{(1)}(x, t) = W_0 \cos(x/L) \cos \omega t$, exhibits an even more intriguing time dependence due to possible spatio-temporal mode matching. In this case

$$S_+ - S_- = 2kx - \frac{4W_0 L v_F \sin(\frac{x}{L})}{\omega^2 L^2 - v_F^2} \times \sin \left[\frac{\omega L + v_F}{2L} t \right] \sin \left[\frac{\omega L - v_F}{2L} t \right]. \quad (18)$$

Now, even when $\omega \rightarrow 0$, the oscillations of j_y persist since the static potential of spatial periodicity L induces a frequency component v_F/L to waves moving at the uniform velocity v_F . This reminds of the ac -Josephson effect [28] where ac -current oscillations are generated by a time-independent voltage. Shifting the phase of the time dependence, $W_2^{(2)}(x, t) = W_0 \cos(x/L) \sin \omega t$ produces

$$S_+ - S_- = 2kx - \frac{2W_0 L \sin(\frac{x}{L})}{\omega^2 L^2 - v_F^2} (\omega L \sin(\frac{v_F t}{L}) - v_F \sin(\omega t)) \quad (19)$$

which vanishes when $\omega \rightarrow 0$. If spatio-temporal matching occurs, i.e. if $\omega \rightarrow v_F/L$, then both of the previous solutions vary proportional to t as $2kx \mp t W_0 \sin \frac{x}{L} \left\{ \begin{smallmatrix} \sin \omega t \\ \cos \omega t \end{smallmatrix} \right\}$ for $\left\{ \begin{smallmatrix} \cos \omega t \\ \sin \omega t \end{smallmatrix} \right\}$ potentials. This results in an amplification of oscillations of j_y with time for relatively small W_0 , Fig. 1c. Indeed, even for small amplitudes of the scalar potentials, the oscillations grow resonantly at times $t \sim 2\pi/W_0$. We mention the analogy to the resonance excitation of plasmonic oscillations (Wood's anomaly [29]) by spatio-temporal matching of the incident light with the grating period.

Concluding, we derived the exact solution of the Dirac equation for electrons in graphene moving strictly perpendicular to a scalar barrier $U(x, t)$, taken as homogeneous along the y -direction, which may vary arbitrarily with time and x . We still find unit transmission probability, referred to as Klein tunneling, rendering at most

a phase to the wave function. Importantly, we discover a nonzero current component j_y parallel to the barrier, despite of vanishing incident momentum p_y . This current arises in valley polarized situations for packets containing both, left and right moving waves. It exhibits striking resemblance to the Josephson current of coupled superconductors and we have shown conditions under which Shapiro step like solutions arise.

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- [1] K.S. Novoselov *et al.*, Nature **438**, 197 (2005).
 - [2] A.H. Castro Neto *et al.*, Rev. Mod. Phys. **81**, 109 (2009).
 - [3] M.I. Katsnelson, K.S. Novoselov, A.K. Geim, Nature Phys. **2**, 620 (2006).
 - [4] N. Stander, B. Huard, D. Goldhaber-Gordon, Phys. Rev. Lett. **102**, 026807 (2009); A.F. Young, P. Kim, Nature Phys. **5**, 222 (2009).
 - [5] C.X. Bai, X.D. Zhang, Phys. Rev. B **76** 075430 (2007); C.H. Park *et al.*, Nature Physics **4**, 213 (2008); C.H. Park *et al.*, Phys. Rev. Lett. **101**, 126804 (2008); M. Barbier, P. Vasilopoulos, F. M. Peeters, Phys. Rev B **81**, 075438 (2010); L.Z. Tan, C.H. Park, S.G. Louie, Phys. Rev. B **81**, 195426 (2010).
 - [6] Y.P. Bliokh *et al.*, Phys. Rev. B **79** 075123 (2009).
 - [7] V.V. Cheianov, V. Fal'ko, B. L. Altshuler, Science **315**, 1252 (2007); V.A. Yampol'skii, S. Savel'ev, F. Nori, New J. Phys. **10**, 053024 (2008).
 - [8] M. Barbier, P. Vasilopoulos, F. M. Peeters, Phys. Rev B **80**, 205415 (2009).
 - [9] H.L. Calvo *et al.*, Appl. Phys. Lett. **98**, 232103 (2011).
 - [10] S.E. Savel'ev, A.S. Alexandrov, Phys. Rev. B in press (2011); arXiv:1103.5983 (2011).
 - [11] M.V. Fistul, K.B. Efetov, Phys. Rev. Lett. **98**, 256803 (2007).
 - [12] H.-Y. Chiu *et al.*, Nano Lett. **10**, 4634 (2010); M.Y. Han *et al.*, Phys. Rev. Lett. **98**, 206805 (2007); B. Huard *et al.*, Phys. Rev. Lett. **98**, 236803 (2007); B. Özyilmaz *et al.*, Phys. Rev. Lett. **99**, 166804 (2007); J.R. Williams, L. DiCarlo, C.M. Marcus, Science **317**, 638 (2007).
 - [13] T.K. Ghosh *et al.*, Phys. Rev. B **77**, 081404(R) (2008); W. Häusler *et al.*, Phys. Rev. B **78**, 165402 (2008); W. Häusler, R. Egger, Phys. Rev. B **80**, 161402(R) (2009).
 - [14] C.L. Kane, E.J. Mele, Phys. Rev. Lett. **95**, 226801 (2005).
 - [15] C.W.J. Beenakker, Rev. Mod. Phys. **80**, 1337 (2008)
 - [16] A. Rycerz, J. Tworzydło, C.W.J. Beenakker, Nature Physics **3**, 172 (2007).
 - [17] S.A. Wolf *et al.*, Science **294**, 1488 (2001).
 - [18] A.R. Akhmerov *et al.*, Phys. Rev. B **77**, 205416 (2008).
 - [19] J.M. Pereira *et al.*, J. Phys.: Condens. Matter **21**, 045301 (2009).
 - [20] J.L. Garcia-Pomar, A. Cortijo, M. Nieto-Vesperinas, Phys. Rev. Lett. **100**, 236801 (2008).
 - [21] A. Hill, A. Sinner, K. Ziegler, New J. Phys. **13**, 035023

- (2011).
- [22] T. Ando, T. Nakanishi, R. Saito, J. Phys. Soc. Jpn. **67**, 2857 (1998).
 - [23] V.V. Cheianov, V.I. Fal'ko, Phys. Rev. B **74**, 041403(R) (2006).
 - [24] P.G. Silvestrov, K.B. Efetov, Phys. Rev. Lett. **98**, 016802 (2007).
 - [25] S.V. Syzranov, M.V. Fistul, K.B. Efetov, Phys. Rev. B **78**, 045407 (2008).
 - [26] B. Trauzettel, Ya.M. Blanter, A.F. Morpurgo, Phys. Rev. B **75**, 035305 (2007).
 - [27] R. Courant and D. Hilbert, *Methods of Mathematical Physics*, Volume II, Wiley-Interscience (1962).
 - [28] M. Tinkham, *Introduction to Superconductivity*, Dover Publications Inc. (2004).
 - [29] H. Raether, *Surface Plasmons*, Springer, New York (1988).